

APPENDIX:
CHEMICAL VOLATILIZATION DATABASE

Equations to Solve Mass Transfer Parameters in Database

General Equations Applied to All Applicable Sources:

<p>Chemical Stripping Efficiency = $\eta = \left(1 - \frac{C_i}{C_{i,in}}\right) \times 100\%$</p> <p>Mass Closure Estimate = $\% \text{ mass rec overd} = \frac{V_l C_{l,2} + V_g C_{g,2} + Q_v \int_{t_1}^{t_2} C_{l,t} dt}{V_l C_{l,1} + V_g C_{g,1}}$</p>	<p>Variables</p> <p>C_i = chemical concentration in liquid phase out of system $C_{i,in}$ = chemical concentration in liquid phase entering system</p> <p>V_l = liquid volume $C_{l,1}$ = chemical concentration in liquid phase at time 1 $C_{l,2}$ = chemical concentration in liquid phase at time 2 V_g = headspace volume $C_{g,1}$ = chemical concentration in gas phase at time 1 $C_{g,2}$ = chemical concentration in gas phase at time 2 Q_v = ventilation rate of system t_1 = time 1 t_2 = time 2</p>	<p>Units</p> <p>mg/L mg/L</p> <p>L mg/L mg/L</p> <p>L mg/L mg/L</p> <p>L/min min</p> <p>min</p>																																				
k_g/k_l Matrix Method																																						
<table border="1" style="margin: auto;"> <thead> <tr> <th>$K_l A_j$</th> <th>Chemical 1</th> <th>Chemical 2</th> <th>Chemical 3</th> <th>Chemical 4</th> <th>Chemical n</th> </tr> </thead> <tbody> <tr> <td>$K_l A_i$</td> <td>1</td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Chemical 2</td> <td></td> <td>1</td> <td></td> <td></td> <td></td> </tr> <tr> <td>Chemical 3</td> <td></td> <td></td> <td>1</td> <td></td> <td></td> </tr> <tr> <td>Chemical 4</td> <td></td> <td></td> <td></td> <td>1</td> <td></td> </tr> <tr> <td>Chemical n</td> <td></td> <td></td> <td></td> <td></td> <td>1</td> </tr> </tbody> </table>	$K_l A_j$	Chemical 1	Chemical 2	Chemical 3	Chemical 4	Chemical n	$K_l A_i$	1					Chemical 2		1				Chemical 3			1			Chemical 4				1		Chemical n					1	<p>Variables</p> <p>$K_l A_i$ = overall mass transfer value for chemical "i" $K_l A_j$ = overall mass transfer value for chemical "j" $\Psi_i = (D_l/D_g)^{n/2}$ D_l = liquid-phase diffusion coefficient for chemical "i" D_g = liquid-phase diffusion coefficient for chemical "j" n = liquid-phase power constant $\Psi_g = (D_g/D_l)^{n/2}$ D_g = gas-phase diffusion coefficient for chemical "i" D_l = gas-phase diffusion coefficient for chemical "j" n_t = liquid-phase power constant H_{ci} = Henry's law constant for chemical "i" H_{cj} = Henry's law constant for chemical "j" k_{gj}/k_{li} = ratio of liquid- and gas-phase mass transfer coefficients for chemical "j"</p>	<p>Units</p> <p>L/min L/min</p> <p>cm²/sec cm²/sec</p> <p>cm²/sec cm²/sec</p> <p>liquid-phase power constant</p> <p>cm²/sec cm²/sec</p> <p>liquid-phase power constant</p> <p>$m^3_{\text{liq}}/m^3_{\text{gas}}$ $m^3_{\text{liq}}/m^3_{\text{gas}}$</p>
$K_l A_j$	Chemical 1	Chemical 2	Chemical 3	Chemical 4	Chemical n																																	
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Three $n \times n$ matrices were filled with the following values:																																						
Matrix 1: Ratio of measured $K_l A_i/K_l A_j$ values for all chemicals and single experimental condition																																						
Matrix 2: Ratio of predicted $K_l A_i/K_l A_j$ values for all chemicals using an assumed k_g/k_l value in the following equation:																																						
$\frac{K_l A_i}{K_l A_j} = \Psi_i \Psi_g \left(\frac{H_{ci}}{H_{cj}} \right) \left\{ \frac{1 + \left[\frac{k_{gi}}{k_{lj}} \right] H_{ej}}{\Psi_i + \Psi_g H_{ci} \left[\frac{k_{gi}}{k_{lj}} \right]} \right\}$																																						
Matrix 3: Normalized residual between values in corresponding cells of Matrix 1 and Matrix 2. Each column and row of this matrix was added to find the total residual to be minimized. The value of k_g/k_l used to predict $K_l A$ values in Matrix 2 was used to minimize total residual. Minimum residual value corresponded to "best" k_g/k_l value.																																						
Use k_g/k_l value and $\frac{1}{K_l A} = \frac{1}{k_l A} + \frac{1}{k_g A \bullet H_c}$ to solve for liquid-phase mass transfer coefficient ($k_l A$) and gas-phase mass transfer coefficient ($k_g A$)																																						

Solution Methods for Values of $K_L A$ Referenced in Database

Method

1	<p>Applicable Sources: Shower, Flow-through Bathtub</p> <p>Model Equation: $C_{l,out} = C_{l,in} \exp\left(-\frac{K_L A}{Q_l}\right) + \left(\frac{C_g}{H_c}\right)\left(1 - \exp\left(-\frac{K_L A}{Q_l}\right)\right)$</p> <p>Predicts $C_{l,out}$</p> <p>Solution Technique: Solve for $K_L A$ by minimizing normalized residual between measured $C_{l,out}$ and predicted $C_{l,out}$:</p>	<p>Variables</p> <table border="0"> <tbody> <tr> <td>$C_{l,out}$ =</td><td>chemical concentration in liquid-phase exiting system</td><td>Units mg/L</td></tr> <tr> <td>$C_{l,in}$ =</td><td>chemical concentration in liquid-phase entering system</td><td>mg/L</td></tr> <tr> <td>$K_L A$ =</td><td>overall mass transfer coefficient multiplied by interfacial area</td><td>L/min</td></tr> <tr> <td>Q_l =</td><td>system liquid flowrate</td><td>L/min</td></tr> <tr> <td>C_g =</td><td>chemical concentration in gas-phase of system at time t</td><td>mg/L</td></tr> <tr> <td>H_c =</td><td>Henry's law coefficient of chemical</td><td>(L_{liq}/L_{gas})</td></tr> </tbody> </table>	$C_{l,out}$ =	chemical concentration in liquid-phase exiting system	Units mg/L	$C_{l,in}$ =	chemical concentration in liquid-phase entering system	mg/L	$K_L A$ =	overall mass transfer coefficient multiplied by interfacial area	L/min	Q_l =	system liquid flowrate	L/min	C_g =	chemical concentration in gas-phase of system at time t	mg/L	H_c =	Henry's law coefficient of chemical	(L _{liq} /L _{gas})
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A-3

2	<p>Applicable Sources: Shower, Flow-through Bathtub</p> <p>Model Equation: $C_g = \frac{a}{b} + \left(C_{g,in} - \frac{a}{b}\right) \exp(-bt)$</p> <p>Predicts C_g</p> <p>where:</p> $a = \frac{\left(Q_l C_{l,in} \left(1 - \exp\left(-\frac{K_L A}{Q_l}\right)\right) + Q_g C_{g,in}\right)}{V_g}$ $b = \frac{\left(\frac{Q_l}{H_c}\right) \left[\left(1 - \exp\left(-\frac{K_L A}{Q_l}\right)\right) + Q_g\right]}{V_g}$ <p>Solution Technique: Solve for $K_L A$ by minimizing normalized residual between measured C_g and predicted C_g:</p>	<p>Variables</p> <table border="0"> <tbody> <tr> <td>C_g =</td><td>chemical concentration in gas-phase</td><td>Units mg/L</td></tr> <tr> <td>$C_{g,in}$ =</td><td>chemical concentration in gas-phase at start of experiment</td><td>mg/L</td></tr> <tr> <td>Q_l =</td><td>system liquid flowrate</td><td>L/min</td></tr> <tr> <td>$C_{l,in}$ =</td><td>chemical concentration in liquid-phase entering system</td><td>mg/L</td></tr> <tr> <td>$K_L A$ =</td><td>overall mass transfer coefficient multiplied by interfacial area</td><td>L/min</td></tr> <tr> <td>Q_g =</td><td>system ventilation rate</td><td>L/min</td></tr> <tr> <td>V_g =</td><td>headspace volume</td><td>L</td></tr> <tr> <td>H_c =</td><td>Henry's law constant of chemical</td><td>(L_{liq}/L_{gas})</td></tr> </tbody> </table>	C_g =	chemical concentration in gas-phase	Units mg/L	$C_{g,in}$ =	chemical concentration in gas-phase at start of experiment	mg/L	Q_l =	system liquid flowrate	L/min	$C_{l,in}$ =	chemical concentration in liquid-phase entering system	mg/L	$K_L A$ =	overall mass transfer coefficient multiplied by interfacial area	L/min	Q_g =	system ventilation rate	L/min	V_g =	headspace volume	L	H_c =	Henry's law constant of chemical	(L _{liq} /L _{gas})
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3

Applicable Sources: Washing Machine Fill Cycle, Filling Bathtub

Model Equations:

Predicts C_l and C_g

Discretized Equations:

$$C_l^{n+1} = \left[\frac{Q_l C_{l,in}}{V_l^n} - \frac{Q_l C_l^n}{V_l^n} - \frac{K_L A C_l^n}{V_l^n} + \frac{K_L A C_g^n}{V_l^n H_c} \right] \Delta t + C_l^n$$

$$C_g^{n+1} = \left[\frac{-Q_g C_g^n}{(V_t - V_l^n)} + \frac{Q_l C_g^n}{(V_t - V_l^n)} + \frac{K_L A C_l^n}{(V_t - V_l^n)} - \frac{K_L A C_g^n}{(V_t - V_l^n) H_c} \right] \Delta t + C_g^n$$

Variables	Units
C_l^n = chemical concentration in liquid phase at time step n	mg/L
C_l^{n+1} = chemical concentration in liquid phase at time step n+1	mg/L
V_l^n = liquid volume at time step n	L
V_t = total volume of system	L
$K_L A$ = overall mass transfer coefficient multiplied by interfacial area	L/min
Q_l = system liquid flowrate	L/min
$C_{l,in}$ = chemical concentration in liquid-phase entering system	mg/L
H_c = Henry's law constant of chemical	(L _{liq} /L _{gas})
C_g^n = chemical concentration in gas phase at time step n	mg/L
C_g^{n+1} = chemical concentration in gas phase at time step n+1	mg/L
Q_g = system ventilation rate	L/min
Δt = differential time step	min

2nd Order Runge-Kutta Technique:

$$C^{n+1} = C^n + \frac{\Delta t}{2} \left\{ f(t^n, C^n) + f\left[t^n + \Delta t, C^n + \Delta t f(t^n, C^n)\right] \right\}$$

Solution Technique: Solve for $K_L A$ by minimizing normalized residual between measured C_l^{n+1} or C_g^{n+1} and predicted values at associated time steps.
Note: Liquid-phase concentration equation is dependent on gas-phase concentration

$$\left[\frac{(C_{l,measured} - C_{l,predicted})}{C_{l,measured}} \right]^2$$

4

Applicable Sources: Dishwasher, Washing Machine Wash/Rinse Cycle, Handwashing Dishes in Kitchen Sink, Bathing

Model Equation: $C_l = C_{l,0} \left[\exp \left(-\frac{D}{2} t \right) \cosh \left(\left(\sqrt{\frac{D^2}{4} - E} \right) t \right) \right] + \left(\frac{BF}{Z} + \frac{EC_{l,0}}{Z} - \frac{DC_{l,0}}{2} \right) \left[\frac{1}{\left(\sqrt{\frac{D^2}{4} - E} \right)} \exp \left(-\frac{D}{2} t \right) \sinh \left(\left(\sqrt{\frac{D^2}{4} - E} \right) t \right) \right]$

Predicts C_l

where:

$$Z = \frac{K_L A}{V_l}$$

$$B = \frac{K_L A}{V_l H_c}$$

$$X = \frac{K_L A}{V_g}$$

$$Y = \frac{Q_g}{V_g} + \frac{K_L A}{V_g H_c}$$

$$D = Z + Y$$

$$E = ZY - BX$$

$$F = ZC_{g,0} + XC_{l,0}$$

Variables	Units
C_l = chemical concentration in liquid phase	mg/L
$C_{l,0}$ = initial chemical concentration in liquid phase	mg/L
$K_L A$ = overall mass transfer coefficient multiplied by interfacial area	L/min
V_l = system liquid volume	L
H_c = Henry's law constant of chemical	(L _{liq} /L _{gas})
V_g = system headspace volume	L
Q_g = system ventilation rate	L/min
$C_{g,0}$ = initial chemical concentration in gas phase	mg/L
t = time	min

Solution Technique: Solve for $K_L A$ by minimizing residual between measured C_l and predicted C_l :

$$\left[\frac{(C_{l,measured} - C_{l,predicted})}{C_{l,measured}} \right]^2$$

5 **Applicable Sources:** Dishwasher, Washing Machine Wash/Rinse Cycle, Handwashing Dishes in Kitchen Sink, Bathing

Model Equation: Predicts C_g

$$C_g = C_{g,0} \exp\left(-\frac{D}{2}t\right) \cosh\left(\left(\sqrt{\frac{D^2}{4} - E}\right)t\right) + \left(F - \frac{DC_{g,0}}{2}\right) \left[\frac{1}{\left(\sqrt{\frac{D^2}{4} - E}\right)} \exp\left(-\frac{D}{2}t\right) \sinh\left(\left(\sqrt{\frac{D^2}{4} - E}\right)t\right) \right]$$

where: $Z = \frac{K_L A}{V_l}$ $B = \frac{K_L A}{V_l H_c}$ $X = \frac{K_L A}{V_g}$

$$Y = \frac{Q_g}{V_g} + \frac{K_L A}{V_g H_c} \quad D = Z + Y \quad E = ZY - BX$$

$$F = ZC_{g,0} + XC_{l,0}$$

Variables

		Units
C_g =	chemical concentration in gas phase	mg/L
$C_{g,0}$ =	initial chemical concentration in gas phase	mg/L
$K_L A$ =	overall mass transfer coefficient multiplied by interfacial area	L/min
V_l =	system liquid volume	L
H_c =	Henry's law constant of chemical	(L _{liq} /L _{gas})
V_g =	system headspace volume	L
Q_g =	system ventilation rate	L/min
$C_{l,0}$ =	initial chemical concentration in liquid phase	mg/L
t =	time	min

Solution Technique: Solve for $K_L A$ by minimizing residual between measured C_g and predicted C_g :

$$\left[\frac{(C_{g, \text{measured}} - C_{g, \text{predicted}})}{C_{g, \text{measured}}} \right]^2$$

6 **Applicable Sources:** Kitchen Sink (with recirculating batch reactor experimental design)

Model Equation: Predicts C_l

$$C_l = C_{l,0} \exp(-K_L a t)$$

Variables

		Units
C_l =	chemical concentration in liquid phase at time t	mg/L
$C_{l,0}$ =	initial chemical concentration in liquid phase	mg/L
$K_L a$ =	overall mass transfer coefficient multiplied by interfacial area/liquid volume	min ⁻¹
t =	time	min

Solution Technique: Slope of best curve fit of $\ln(C_l/C_{l,0})$ vs. time equal to $K_L a$

Chemical stripping efficiencies also solved using best fit equation to measured liquid data according to:

$$C_l = C_{l,0} \exp\left(-\frac{t}{\theta_{ii}} \eta\right)$$

SHOWER DATABASE

STUDY: Moya, J, Howard-Reed, C, and Corsi, R.L
Study year: 1999
Reference: *Environmental Science and Technology*, Vol. 33, 1999, pp. 2321-2327
Solution Methods: Method 1 for acetone, ethyl acetate, toluene, ethylbenzene, cyclohexane
Assumptions: None
Comments: Values of η and $K_L A$ are averages of values determined for three separate time periods within experiment.
Mass closure based on liquid standard curve created using well-dissolved tracer bag.

* = Could not be determined with available data; n/m = not measured.

Entry #	Operating Conditions		Chemical Properties				Chemical Concentrations				Mass Transfer Parameters					
			H_c @ 21 C (m ³ _{liq} /m ³ _{gas})	D_l @ 24 C (cm ² /sec)	D_g @ 24 C (cm ² /sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	K_g/k_l	Mass Closure (%)	
1	spray type = coarse	duration (min) = 8	chemical	0.0010×10^{-5}	0.11	38	34 - 37	0	0.036	6.3	1.8	13	1986	153	99	
	Liquid Temperature (C) = 21		Acetone	0.0010	1.1×10^{-5}	0.11	38	34 - 37	0	0.036	6.3	1.8	13	1986	153	99
	Liquid Flowrate (L/min) = 9.1		Ethyl Acetate	0.0042	9.5×10^{-6}	0.092	26	20 - 24	0	0.068	15	2.9	7.3	1111	153	100
	Gas Flowrate (L/min) = 370		Toluene	0.24	9.1×10^{-6}	0.085	4.5	1.8	0	0.041	61	8.8	9	1380	153	90
	Shower Stall Volume (L) = 1745		Ethylbenzene	0.27	8.4×10^{-6}	0.077	6.1	2.3	0	0.029	62	8.9	9.1	1395	153	77
	Person Present = No		Cyclohexane	6.5	9.0×10^{-6}	0.088	1.8	0.63	0	0.0069	65	9.6	9.6	1468	153	78
2	spray type = fine	duration (min) = 8	chemical	0.0011×10^{-5}	0.11	42	35 - 40	0	0.041	8.4	3.0	16	3519	223	97	
	Liquid Temperature (C) = 22		Acetone	0.0011	1.1×10^{-5}	0.11	42	35 - 40	0	0.041	8.4	3.0	16	3519	223	97
	Liquid Flowrate (L/min) = 9.1		Ethyl Acetate	0.0044	9.5×10^{-6}	0.092	22	16 - 20	0	0.081	15	4.0	8.1	1807	223	104
	Gas Flowrate (L/min) = 343		Toluene	0.25	9.1×10^{-6}	0.085	7.0	2.3	0	0.057	68	11	11	2434	223	82
	Shower Stall Volume (L) = 1745		Ethylbenzene	0.27	8.4×10^{-6}	0.077	7.3	2.3	0	0.032	68	11	11	2384	223	66
	Person Present = No		Cyclohexane	6.6	9.0×10^{-6}	0.088	3.3	0.88	0	0.0097	73	12	12	2652	223	68
3	spray type = coarse	duration (min) = 8	chemical	0.0010×10^{-5}	0.11	42	36 - 39	0	0.035	9.1	1.4	8.6	1723	200	98	
	Liquid Temperature (C) = 21		Acetone	0.0010	1.1×10^{-5}	0.11	42	36 - 39	0	0.035	9.1	1.4	8.6	1723	200	98
	Liquid Flowrate (L/min) = 6.1		Ethyl Acetate	0.0044	9.5×10^{-6}	0.092	26	19 - 22	0	0.057	20	2.3	5.1	1030	200	98
	Gas Flowrate (L/min) = 360		Toluene	0.24	9.1×10^{-6}	0.085	7.0	2.6	0	0.029	63	6.2	6.4	1274	200	82
	Shower Stall Volume (L) = 1745		Ethylbenzene	0.26	8.4×10^{-6}	0.077	7.5	2.8	0	0.011	63	6.0	6.2	1234	200	64
	Person Present = No		Cyclohexane	6.3	9.0×10^{-6}	0.088	3.0	1.0	0	0.0079	66	6.5	6.5	1305	200	77
4	spray type = fine	duration (min) = 8	chemical	0.0011×10^{-5}	0.11	43	37 - 41	0	0.037	9.3	1.5	8.8	1720	195	98	
	Liquid Temperature (C) = 22		Acetone	0.0011	1.1×10^{-5}	0.11	43	37 - 41	0	0.037	9.3	1.5	8.8	1720	195	98
	Liquid Flowrate (L/min) = 6.1		Ethyl Acetate	0.0044	9.5×10^{-6}	0.092	31	22 - 26	0	0.083	20	2.5	5.3	1031	195	101
	Gas Flowrate (L/min) = 360		Toluene	0.25	9.1×10^{-6}	0.085	6.1	2.2	0	0.036	64	6.4	6.5	1275	195	92
	Shower Stall Volume (L) = 1745		Ethylbenzene	0.28	8.4×10^{-6}	0.077	5.5	2.0	0	0.018	63	6.2	6.3	1232	195	76
	Person Present = No		Cyclohexane	6.7	9.0×10^{-6}	0.088	2.0	0.67	0	0.0063	66	6.7	6.7	1309	195	85

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
		H _c @ 35 C Chemical	D _l @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _g A (L/min)	k _g /k _l	Mass Closure (%)	
5	Spray Type = coarse														
	Duration (min) = 8														
	Liquid Temperature (C) = 35	Acetone	0.0022	1.1 x 10 ⁻⁵	0.11	42	34 - 38	0	0.077	13	2.8	14	1548	111	97
	Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0077	9.5 x 10 ⁻⁶	0.092	24	16 - 19	0	0.13	27	5.5	12	1322	111	102
	Gas Flowrate (L/min) = 379	Toluene	0.37	9.1 x 10 ⁻⁶	0.085	6.4	2.0	0	0.056	68	11	11	1223	111	77
	Shower Stall Volume (L) = 1745	Ethylbenzene	0.54	8.4 x 10 ⁻⁶	0.077	8.0	2.5	0	0.032	68	11	11	1188	111	68
	Person Present = No	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	2.6	0.63	0	0.0093	75	13	13	1439	111	66
6	Spray Type = fine														
	Duration (min) = 8														
	Liquid Temperature (C) = 34	Acetone	0.0021	1.1 x 10 ⁻⁵	0.11	40	34 - 38	0	0.071	11	3.4	16	2095	131	99
	Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0074	9.5 x 10 ⁻⁶	0.092	24	15 - 18	0	0.12	28	6.9	14	1852	131	100
	Gas Flowrate (L/min) = 354	Toluene	0.35	9.1 x 10 ⁻⁶	0.085	5.3	1.3	0	0.053	75	13	14	1776	131	94
	Shower Stall Volume (L) = 1745	Ethylbenzene	0.51	8.4 x 10 ⁻⁶	0.077	4.6	1.1	0	0.031	75	13	13	1708	131	81
	Person Present = No	Cyclohexane	9.6	9.0 x 10 ⁻⁶	0.088	1.6	0.35	0	0.0054	77	14	14	1786	131	74
7	Spray Type = fine														
	Duration (min) = 8														
	Liquid Temperature (C) = 34	Acetone	0.0021	1.1 x 10 ⁻⁵	0.11	40	32 - 37	0	0.071	12	3.7	15	2316	153	99
	Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0074	9.5 x 10 ⁻⁶	0.092	25	15 - 19	0	0.13	29	6.7	13	1945	153	102
	Gas Flowrate (L/min) = 373	Toluene	0.36	9.1 x 10 ⁻⁶	0.085	5.2	1.3	0	0.058	74	12	13	1930	153	90
	Shower Stall Volume (L) = 1745	Ethylbenzene	0.52	8.4 x 10 ⁻⁶	0.077	3.8	1.0	0	0.031	74	12	12	1855	153	78
	Person Present = No	Cyclohexane	9.8	9.0 x 10 ⁻⁶	0.088	0.71	0.17	0	0.0065	77	13	13	1950	153	85
8	Spray Type = coarse														
	Duration (min) = 8														
	Liquid Temperature (C) = 36	Acetone	0.0024	1.1 x 10 ⁻⁵	0.11	41	32 - 36	0	0.054	16	2.2	11	1169	110	96
	Liquid Flowrate (L/min) = 6.1	Ethyl Acetate	0.0080	9.5 x 10 ⁻⁶	0.092	24	14 - 17	0	0.081	32	3.8	8.2	901	110	99
	Gas Flowrate (L/min) = 364	Toluene	0.38	9.1 x 10 ⁻⁶	0.085	5.6	1.5	0	0.036	74	8.4	8.6	949	110	98
	Shower Stall Volume (L) = 1745	Ethylbenzene	0.57	8.4 x 10 ⁻⁶	0.077	5.3	1.4	0	0.023	73	8.2	8.3	917	110	86
	Person Present = No	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	1.9	0.46	0	0.0054	76	8.6	8.6	943	110	77
9	Spray Type = fine														
	Duration (min) = 8														
	Liquid Temperature (C) = 35	Acetone	0.0022	1.1 x 10 ⁻⁵	0.11	42	33 - 37	0	0.079	14	2.3	9.6	1380	143	102
	Liquid Flowrate (L/min) = 6.1	Ethyl Acetate	0.0077	9.5 x 10 ⁻⁶	0.092	24	14 - 18	0	0.12	33	4.7	9.0	1292	143	108
	Gas Flowrate (L/min) = 371	Toluene	0.36	9.1 x 10 ⁻⁶	0.085	6.0	1.6	0	0.048	73	8.1	8.3	1189	143	88
	Shower Stall Volume (L) = 1745	Ethylbenzene	0.53	8.4 x 10 ⁻⁶	0.077	5.6	1.5	0	0.029	72	7.9	8.0	1139	143	92
	Person Present = No	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	1.8	0.43	0	0.0060	75	8.4	8.4	1203	143	81

10	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type =	fine	Chemical	H _c @ 34 C (m ³ _{liq} /m ³ _{gas})	D _l @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{L,A} (L/min)	k _A (L/min)	k _{g,A} (L/min)	k _g /k _I	Mass Closure (%)
Spray Type =	fine															
Duration (min) =	8															
Liquid Temperature (C) =	34		Acetone	0.0021	1.1 x 10 ⁻⁵	0.11	40	32 - 37	0	0.081	15	2.5	11	1507	138	103
Liquid Flowrate (L/min) =	6.1		Ethyl Acetate	0.0074	9.5 x 10 ⁻⁶	0.092	24	14 - 16	0	0.13	36	5.3	10	1443	138	106
Gas Flowrate (L/min) =	367		Toluene	0.36	9.1 x 10 ⁻⁶	0.085	5.4	1.3	0	0.047	77	9.2	9.3	1291	138	88
Shower Stall Volume (L) =	1745		Ethylbenzene	0.53	8.4 x 10 ⁻⁶	0.077	4.5	1.1	0	0.027	75	8.8	8.9	1227	138	75
Person Present =	No		Cyclohexane	9.9	9.0 x 10 ⁻⁶	0.088	0.84	0.17	0	0.0057	80	9.9	9.9	1366	138	80

STUDY: Keating, McKone, and Gillett

Study year: 1997

Atmospheric Environment, Vol. 31, No. 2, 1997, pp. 123-130

Solution Methods:

Assumptions: $C_{q,\text{in}} = 0$

Comments: Current values picked off graph presented in paper

$C_{g, \text{end}}$ values picked on graph presented in paper.

Resulting measurements at each sample location, respectively, were not found to be statistically different, as values listed are averages for three sample times.

Results for studies 11, 12, 14, and 16 are based on three different experiments.

Results for studies 11, 12, 14, and 16 are based on three different experiments. Results for studies 13 and 15 are based on two different experiments. (Individual results not given in paper — only averages.)

Results for studies 13 and 15 are based on two different experiments. (Individual results not given in paper.) Liquid flowrate value of 3.5 l/min is average of range of values given in paper (3.1 l/min to 3.8 l/min).

* = Could not be determined with available data; n/m = not measured

STUDY:	Giardino and Andelman
Study year:	1996
Reference:	<i>Journal of Exposure Analysis and Environmental Epidemiology</i> , Vol. 6, No. 4, 1996, pp. 413-423
Solution Method:	Method 1
Assumptions:	$C_{g,in} = 0.$ No $C_{l,out}$ values were reported; assumed it was equal to $(1-\eta) \times C_{l,in}$, where η is given in paper. $C_{l,out}$ remained relatively constant for entire experiment.
Comments:	$C_{l,in}$ is reported average value for 10-minute experiment. Thus, η is an average value for 10-min

* = Could not be determined with available data; n/m = not measured.

— could not be determined with available data; n/m = not measured.

Reaction Conditions

STUDY: Giardino and Hageman
Study year: 1996
Reference: *Environmental Science and Technology*, Vol. 30, No. 4, 1996, pp.1242-1244
Solution Method: Method 1
Assumptions: No $C_{i,out}$ values were reported; assumed it was equal to $(1-\eta) \times C_{i,in}$ where η is given in paper.

The reported value of η is an average value based on pairs of influent and effluent liquid samples taken during experiment.

$$D_{Rn} = \left(\frac{MW_{solvent}}{MW_{solute}} \right)^{0.5}$$

$$\frac{D_{l,Rn}}{D_{l,toluene}} = \left(\frac{MW_{toluene}}{MW_{Rn}} \right)^{0.5}$$

* = Could not be determined with available data; n/m = not measured.

STUDY:	Bernhardt and Hess
Study year:	1995
Reference:	Bernhardt's Master's Thesis for The University of Maine
Solution Method:	Method 1
Assumptions:	<p>Shower stall and bathroom volumes were not given, so assumed a typical bathroom volume of 10000 L.</p> <p>Shower curtain open for all experiments; thus used bathroom volume for V_g.</p>
	$Q_g = 0$
	$C_{g,in} = 0$
Comments:	<p>Exact water temperature not given, so assumed $T = 23^\circ\text{C}$ for "cold" water.</p> <p>Liquid-phase diffusion coefficient estimated using relationship given for Giardino and Hageman (1996).</p>

Comments: Liquid-phase diffusion coefficient estimated using relationship given for Giardino and Hageman (1996).

* = Could not be determined with available data; n/m = not measured.

STUDY: Hopke , Raunemaa, Datye, Kuuspalo, and Jensen

Study year: 1995

Reference: In Morawska et al. *Indoor Air: An Integrated Approach*, Elsevier Science Ltd., 1995, pp. 107-110.

Solution Method:

Assumptions:

Comments: Liquid-n

Comments: Liquid-phase diffusion coefficient estimated using relationship given for Gardino and Hagerman (1958). CPM = counts per minute measured with a liquid scintillation counter.

CPM = counts per minute measured with a liquid scintillation counter.
Not enough information given to calculate K₁A or mass closure

Not enough information given to calculate $K_L A$ or mass closure.

* = Could not be determined with available data; n/m = not measured.

STUDY: Keating and McKone
Study year: 1993
Reference: *Modeling of Indoor Air Quality and Exposure, ASTM STP 1205*, 1993, pp. 14-24
Solution Method: Method 1
Assumptions: $C_{g,in} = 0$
Comments: $C_{g,end}$ values visually picked off graph in paper.

Values for each nozzle represent average of three simulations.

* = Could not be determined with available data; n/m = not measured.

STUDY: Giardino, Esmen, and Andelman
Study year: 1992
Reference: *Environmental Science and Technology*, Vol. 26, 1992, pp.1602-1606
Solution Method: N/A
Assumptions: No $C_{l,out}$ values were reported, assumed it was equal to $(1-\eta) \times C_{l,in}$, where η is given in paper.
Comments: Shower had a vertical spray with no water impacting stall walls.
Not enough information given in the paper to calculate $K_L A$ values or mass closure.
Gas-phase concentration reported is average value for entire experiment.

* = Could not be determined with available data; n/m = not measured.

	Operating Conditions	Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
		H _c @ 22 C Chemical	D _l @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{L A} (L/min)	k _A (L/min)	k _{g A} (L/min)	k _{g/k_l}	Mass Clo (%)
57	Spray Type = standard Duration (min) = not given Liquid Temperature (C) = 22 Liquid Flowrate (L/min) = 5 Gas Flowrate (L/min) = 70 Shower Stall Volume (L) = not given Person Present = No	Trichloroethene	0.37	9.4 x 10 ⁻⁶	0.084	0.46	0.15	0	0.025	67	*	*	*	*
58	Spray Type = standard Duration (min) = not given Liquid Temperature (C) = 21 Liquid Flowrate (L/min) = 10 Gas Flowrate (L/min) = 26 Shower Stall Volume (L) = not given Person Present = No	Trichloroethene	0.36	9.4 x 10 ⁻⁶	0.084	0.78	0.32	0	0.080	59	*	*	*	*

STUDY: Tancrede, Yanagisawa, and Wilson
Study year: 1992
Reference: *Atmospheric Environment*, Vol. 26A, No. 6, 1992, pp. 1103-1111
Solution Method: Method 1
Assumptions: C_{g,in} = 0
Comments: C_{l,in} is average of showerhead liquid samples collected at 2, 6, and 11 minutes.
C_{l,out} is average of drain liquid samples collected at 8 and 12 minutes.
One C_g sample was collected at 10 minutes at nose level in the shower stall.

* = Could not be determined with available data; n/m = not measured.

	Operating Conditions	Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
		H _c @ 25 C Chemical	D _l @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{L A} (L/min)	k _A (L/min)	k _{g A} (L/min)	k _{g/k_l}	Mass Clo (%)	
59	Spray Type = unknown Duration (min) = 10 Liquid Temperature (C) = 25 Liquid Flowrate (L/min) = 13.6 Gas Flowrate (L/min) = 34.8 Shower Stall Volume (L) = 1491 Person Present = No	CCl ₄ PCE Trichloroethene Chloroform TCPA	1.2 0.74 0.42 0.17 0.012	9.2 x 10 ⁻⁶ 8.5 x 10 ⁻⁶ 9.4 x 10 ⁻⁶ 9.7 x 10 ⁻⁶ 7.9 x 10 ⁻⁶	0.072 0.077 0.084 0.10 0.073	8.2 x 10 ⁻⁵ 1.1 x 10 ⁻⁴ 0.0016 0.0026 0.092	5.0 x 10 ⁻⁵ 4.9 x 10 ⁻⁵ 6.8 x 10 ⁻⁴ 0 0.073	0 0 0 0 0	1.4 x 10 ⁻⁶ 2.7 x 10 ⁻⁵ 4.9 x 10 ⁻⁵ 7.8 x 10 ⁻⁵ 3.9 x 10 ⁻⁴	39	7.0	7.2	205	29	82
										56	12	13	365	29	345
										58	14	16	446	29	80
										42	11	13	372	29	94
										21	2.5	9.8	281	29	85

60	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type =	unknown	Chemical	H _c @ 33 C (m ³ _{liq} /m ³ _{gas})	D _l @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{LA} (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_l} (%)	Mass Closure (%)
	Duration (min) =	10					1.0 x 10 ⁻⁴	2.5 x 10 ⁻⁵	0	4.6 x 10 ⁻⁶	76	21	22	412	19	78
	Liquid Temperature (C) =	33	CCl ₄	1.7	9.2 x 10 ⁻⁵	0.072										
	Liquid Flowrate (L/min) =	13.5	PCE	1.1	8.5 x 10 ⁻⁶	0.077	2.6 x 10 ⁻⁴	8.6 x 10 ⁻⁵	0	8.3 x 10 ⁻⁶	67	17	17	329	19	72
	Gas Flowrate (L/min) =	34.8	Trichloroethene	0.57	9.4 x 10 ⁻⁶	0.084	0.0031	0.0012	0	1.2 x 10 ⁻⁴	61	15	17	314	19	85
	Shower Stall Volume (L) =	1491	Chloroform	0.26	9.7 x 10 ⁻⁶	0.10	0.0015	7.0 x 10 ⁻⁴	0	5.0 x 10 ⁻⁵	53	14	17	325	19	88
	Person Present =	No	TCPA	0.013	7.9 x 10 ⁻⁶	0.073	0.090	0.071	0	6.6 x 10 ⁻⁴	21	2.7	17	325	19	88

61	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type =	unknown	Chemical	H _c @ 42 C (m ³ _{liq} /m ³ _{gas})	D _l @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{LA} (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_l} (%)	Mass Closure (%)
	Duration (min) =	10					9.4 x 10 ⁻⁵	2.2 x 10 ⁻⁵	0	4.3 x 10 ⁻⁶	77	21	21	371	17	80
	Liquid Temperature (C) =	42	CCl ₄	2.3	9.2 x 10 ⁻⁵	0.072										
	Liquid Flowrate (L/min) =	13.4	PCE	1.6	8.5 x 10 ⁻⁶	0.077	2.4 x 10 ⁻⁴	7.8 x 10 ⁻⁵	0	7.8 x 10 ⁻⁶	68	16	17	293	17	73
	Gas Flowrate (L/min) =	34.8	Trichloroethene	0.78	9.4 x 10 ⁻⁶	0.084	0.0028	0.0010	0	1.3 x 10 ⁻⁴	64	16	17	295	17	93
	Shower Stall Volume (L) =	1491	Chloroform	0.41	9.7 x 10 ⁻⁶	0.10	0.0014	6.7 x 10 ⁻⁴	0	5.6 x 10 ⁻⁵	52	12	14	236	17	97
	Person Present =	No	TCPA	0.017	7.9 x 10 ⁻⁶	0.073	0.089	0.073	0	0.0010	18	3.7	16	282	17	96

62	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type =	unknown	Chemical	H _c @ 43 C (m ³ _{liq} /m ³ _{gas})	D _l @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _{LA} (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_l} (%)	Mass Closure (%)
	Duration (min) =	10					8.1 x 10 ⁻⁵	3.3 x 10 ⁻⁵	0	2.0 x 10 ⁻⁶	59	8.9	9.0	329	36	83
	Liquid Temperature (C) =	43	CCl ₄	2.4	9.2 x 10 ⁻⁵	0.072										
	Liquid Flowrate (L/min) =	9.7	PCE	1.6	8.5 x 10 ⁻⁶	0.077	1.3 x 10 ⁻⁴	4.0 x 10 ⁻⁵	0	3.2 x 10 ⁻⁶	69	12	12	445	36	73
	Gas Flowrate (L/min) =	34.8	Trichloroethene	0.79	9.4 x 10 ⁻⁶	0.084	0.0018	5.5 x 10 ⁻⁴	0	5.5 x 10 ⁻⁵	69	13	13	483	36	83
	Shower Stall Volume (L) =	1491	Chloroform	0.42	9.7 x 10 ⁻⁶	0.10	0.0025	9.2 x 10 ⁻⁴	0	7.5 x 10 ⁻⁵	63	12	12	446	36	88
	Person Present =	No	TCPA	0.017	7.9 x 10 ⁻⁶	0.073	0.082	0.058	0	8.0 x 10 ⁻⁴	29	4.0	10	377	36	87

STUDY:	Giardino and Andelman
Study year:	1991
Reference:	Poster paper for the Annual Conference of the American Water Works Association, 1991
Solution Method:	Method 1
Assumptions:	$C_{g,in} = 0$
Comments:	All values from Little, J.C. (1992), <i>Environmental Science and Technology</i> , Vol. 26, No. 7, pp. 1341-1349. $C_{l,out}$ is an average value based on reported volatilization value.

* = Could not be determined with available data; n/m = not measured.

STUDY:	McKone and Knezovich
Study year:	1991
Reference:	<i>Journal of the Air and Waste Management Association</i> , Vol. 41, 1991, pp. 282-286
Solution Method:	Method 1
Assumptions:	$C_{g,in} = 0$
Comments:	Studies #66 and #67 based on 4 experiments, respectively. $C_{l,out}$ predicted based on reported average stripping efficiency in paper.

* = Could not be determined with available data; n/m = not measured.

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STUDY:	Jo, Weisel, and Lioy
Study year:	1990
Reference:	Risk Analysis, Vol. 10, No.4, 1990, pp. 581-585
Solution Method:	Method 2
Assumptions:	$C_{g,in} = 0$. $Q_g = 0$.
	Assumed shower air concentration increased linearly such that average gas-phase concentration of entire shower event occurred at the midpoint.
Comments:	Experiments were started 2 minutes after starting water through shower nozzle. Gas samples are average value of 10-minute sample collection.

* = Could not be determined with available data; n/m = not measured.

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
		H_c @ 40 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_l A$ (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
Spray Type =	unknown													
Duration (min) =	10													
Liquid Temperature (C) =	40	Chloroform	0.37	9.7×10^{-6}	0.10	0.013	n/m	0	6.9×10^{-5}	*	2.0	*	*	*
Liquid Flowrate (L/min) =	8.7	Chloroform	0.37	9.7×10^{-6}	0.10	0.013	n/m	0	5.8×10^{-5}	*	1.6	*	*	*
Gas Flowrate (L/min) =	0	Chloroform	0.37	9.7×10^{-6}	0.10	0.020	n/m	0	1.2×10^{-4}	*	2.4	*	*	*
Shower Stall Volume (L) =	1666	Chloroform	0.37	9.7×10^{-6}	0.10	0.021	n/m	0	9.09×10^{-5}	*	1.6	*	*	*
Person Present =	No	Chloroform	0.37	9.7×10^{-6}	0.10	0.023	n/m	0	9.0×10^{-5}	*	1.4	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.024	n/m	0	1.2×10^{-4}	*	1.8	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.024	n/m	0	2.0×10^{-4}	*	3.4	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.025	n/m	0	1.7×10^{-4}	*	2.8	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.027	n/m	0	1.7×10^{-4}	*	2.4	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.028	n/m	0	2.0×10^{-4}	*	2.8	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.031	n/m	0	2.0×10^{-4}	*	2.5	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.032	n/m	0	2.3×10^{-4}	*	2.8	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.040	n/m	0	3.3×10^{-4}	*	3.3	*	*	*

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Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
		H_c @ 40 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_l A$ (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
Spray Type =	unknown													
Duration (min) =	10													
Liquid Temperature (C) =	40	Chloroform	0.37	9.7×10^{-6}	0.10	0.022	n/m	0	1.3×10^{-4}	*	2.2	*	*	*
Liquid Flowrate (L/min) =	8.7	Chloroform	0.37	9.7×10^{-6}	0.10	0.023	n/m	0	1.2×10^{-4}	*	1.9	*	*	*
Gas Flowrate (L/min) =	0	Chloroform	0.37	9.7×10^{-6}	0.10	0.025	n/m	0	1.3×10^{-4}	*	2.0	*	*	*
Shower Stall Volume (L) =	1666	Chloroform	0.37	9.7×10^{-6}	0.10	0.029	n/m	0	2.0×10^{-4}	*	2.6	*	*	*
Person Present =	Yes	Chloroform	0.37	9.7×10^{-6}	0.10	0.029	n/m	0	2.3×10^{-4}	*	3.1	*	*	*
		Chloroform	0.37	9.7×10^{-6}	0.10	0.036	n/m	0	3.1×10^{-4}	*	3.6	*	*	*

STUDY: Giardino, Andelman, Borrazzo, and Davidson
Study year: 1988
Reference: *Journal of the Air Pollution Control Association*, Vol. 38, No. 3, 1988, pp. 278-280
Solution Method: Method 1
Assumptions: $C_{g,in} = 0$
 $Q_g = 0$
Comments: $C_{l,out}$ is average value based on volatilization value reported in paper.

* = Could not be determined with available data; n/m = not measured.

70	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
	Spray Type	Duration (min)	Chemical	H_c @ 21 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_l A$ (L/min)	$k_g A$ (L/min)	k_g/k_l
		17													
Liquid Temperature (C) =	21	SF ₆	185	1.02×10^{-5}	*		18	10	0	n/m	44	3.5	*	*	*
Liquid Flowrate (L/min) =	6.0	SF ₆	185	1.02×10^{-5}	*		8.8	5.6	0	n/m	36	2.7	*	*	*
Gas Flowrate (L/min) =	0	SF ₆	185	1.02×10^{-5}	*		18	8.5	0	n/m	52	4.4	*	*	*
Shower Stall Volume (L) =	1100	SF ₆	185	1.02×10^{-5}	*		26	13	0	n/m	51	4.3	*	*	*
Person Present =	No	SF ₆	185	1.02×10^{-5}	*		24	12	0	n/m	48	3.9	*	*	*
		SF ₆	185	1.02×10^{-5}	*		15	9.2	0	n/m	39	3.0	*	*	*
		SF ₆	185	1.02×10^{-5}	*		19	9.4	0	n/m	50	4.2	*	*	*
		SF ₆	185	1.02×10^{-5}	*		20	11	0	n/m	45	3.6	*	*	*

STUDY: Hodgson, Garbesi, Sextro, and Daisey
Study year: 1988
Reference: Lawrence Berkeley Laboratory Report, Contract No. DE-AC03-76SF00098, 1988
Solution Method: Method 1
Assumptions: Assumed entire bathroom including shower stall was well mixed, such that only bathroom measurements were used to predict $K_L A$.
Comments: For Freon-12, used Henry's law constant given in paper, remaining chemical Henry's law constants using Ashworth *et al.* correlations.

* = Could not be determined with available data; n/m = not measured.

71	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type	Duration (min)	Chemical	H_c @ 40 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_l A$ (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
		10														
Liquid Temperature (C) =	40	Freon - 12	32	1.0×10^{-4}	*		0.073	0.010	4.2×10^{-6}	4.3×10^{-5}	86	27	*	*	23	
Liquid Flowrate (L/min) =	13.7	Freon - 11	6.8	9.0×10^{-6}	0.084		0.011	0.0010	4.0×10^{-6}	1.1×10^{-5}	91	33	34	149	4.4	24
Gas Flowrate (L/min) =	51	PCE	1.4	8.5×10^{-6}	0.077		0.018	0.0032	6.0×10^{-6}	2.5×10^{-5}	82	24	28	122	4.4	38
Bathroom Volume (L) =	10900	TCA	1.2	9.0×10^{-6}	0.080		0.0034	5.0×10^{-4}	1.4×10^{-6}	6.6×10^{-5}	85	27	32	140	4.4	43
Person Present =	No	Trichloroethene	0.73	9.4×10^{-6}	0.084		0.0027	4.0×10^{-4}	0	n/m	85	27	35	154	4.4	*

72	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Spray Type	Duration (min)	Chemical	H_c @ 40 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_l A$ (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
		10														
Liquid Temperature (C) =	40	Freon - 12	32	1.0×10^{-4}	*		0.094	0.018	6.6×10^{-6}	6.7×10^{-5}	81	23	*	*	*	30
Liquid Flowrate (L/min) =	13.7	Freon - 11	6.8	9.0×10^{-6}	0.084		0.0094	0.0018	4.5×10^{-6}	1.2×10^{-5}	81	23	*	*	*	37
Gas Flowrate (L/min) =	51	PCE	1.4	8.5×10^{-6}	0.077		0.029	0.0042	3.6×10^{-6}	2.2×10^{-5}	86	27	*	*	*	26
Bathroom Volume (L) =	10900	TCA	1.2	9.0×10^{-6}	0.080		0.0031	8.0×10^{-4}	6.6×10^{-6}	9.6×10^{-5}	74	19	*	*	*	57
Person Present =	Yes	Trichloroethene	0.73	9.4×10^{-6}	0.084		0.0030	4.0×10^{-4}	0	n/m	87	28	*	*	*	*

STUDY:	Hess, Weiffenbach, and Norton
Study year:	1982
Reference:	<i>Environment International</i> , Vol. 8, 1982, pp. 59-66
Solution Method:	N/A
Assumptions:	Stripping efficiency is value reported in paper. No data given to confirm.
Comments:	Stripping efficiency based on four measurements.

Not enough data collected to calculate $K_L A$ or mass closure.

* = Could not be determined with available data; n/m = not measured.

STUDY: Gesell and Prichard
Study year: 1980
Reference: In *Natural Radiation Environment III*, Vol. 2, Houston: Technical Information Center, U.S. Department of Energy, pp. 1347-1363
Solution Method: N/A
Assumptions: Stripping efficiency is value reported in paper. No data given to confirm.
Comments: Liquid-phase diffusion coefficient estimated using relationship given for Giardino and Hageman (1996)
Not enough data collected to calculate $K_t A$ or mass closure.

* = Could not be determined with available data; n/m = not measured.

STUDY: Partridge, Horton, and Sensintaffer
Study year: 1979
Reference: Data in Nazaroff *et al.*, *Health Physics*, Vol. 52, No. 3, 1987, pp. 281-295
Solution Method: N/A
Assumptions: Stripping efficiency is value reported in paper. No data given to confirm.
Comments: Liquid-phase diffusion coefficient estimated using relationship given for Giardino and Hageman (1996).
 Not enough data collected to calculate $K_L A$ or mass closure.

* = Could not be determined with available data; n/m = not measured.

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Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
		Chemical	H_c @ 25 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	$k_p A$ (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
Spray Type =	unknown														
Duration (min) =	not given	Chemical													
Liquid Temperature (C) =	n/m	Radon		4.4	5.2×10^{-6}	*	*	*	*	*	71	*	*	*	
Liquid Flowrate (L/min) =	n/m														
Gas Flowrate (L/min) =	n/m														
Bathroom Volume (L) =	n/m														
Person Present =	No														

BATHTUB DATABASE

STUDY: Howard, C.
Study year: 1998
Reference: Volatilization Rates of Chemicals from Drinking Water to Indoor Air. Ph.D. Dissertation. University of Texas at Austin, May 1988
Solution Methods: Method 1 for ethyl acetate, toluene, ethylbenzene, cyclohexane
Method 2 for acetone
Assumptions: None
Comments: Values of η and $K_L A$ are averages of values determined for three separate time periods within experiment.

* = Could not be determined with available data.

Entry #	Operating Conditions			Chemical Properties				Chemical Concentrations				Mass Transfer Parameters					
				H_c @ 22 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)	
1	Operation = Flow-through	Duration (min) = 8	Liquid Temperature (C) = 22	H_c @ 22 C Acetone	D_l @ 24 C 9.5×10^{-6}	D_g @ 24 C 0.11	52	50	0	0.019	3.8	0.11	2.9	108	37	98	
			Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0044	9.5×10^{-6}	0.092	25	24	0	0.028	6.1	0.64	4.5	168	37	98
			Gas Flowrate (L/min) = 355	Toluene	0.25	9.1×10^{-6}	0.085	4.9	3.6	0	0.019	26	2.9	3.2	117	37	89
			Shower Stall/Bathtub Volume (L) = 1745	Ethylbenzene	0.28	8.4×10^{-6}	0.077	3.9	2.9	0	0.012	27	2.9	3.1	117	37	86
			Person Present = No	Cyclohexane	6.7	9.0×10^{-6}	0.088	0.94	0.68	0	0.0031	28	3.1	3.1	115	37	85
2	Operation = Flow-through	Duration (min) = 8	Liquid Temperature (C) = 23	H_c @ 23 C Acetone	D_l @ 24 C 9.5×10^{-6}	D_g @ 24 C 0.11	40	39	0	0.016	3.1	0.15	3.2	136	43	99	
			Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0046	9.5×10^{-6}	0.092	25	23	0	0.027	4.7	0.49	3.0	126	43	102
			Gas Flowrate (L/min) = 345	Toluene	0.26	9.1×10^{-6}	0.085	6.4	4.9	0	0.019	24	2.4	2.6	111	43	92
			Shower Stall/Bathtub Volume (L) = 1745	Ethylbenzene	0.30	8.4×10^{-6}	0.077	4.9	3.8	0	0.0088	24	2.4	2.6	109	43	88
			Person Present = No	Cyclohexane	6.9	9.0×10^{-6}	0.088	1.4	1.0	0	0.0032	29	2.9	2.9	126	43	88
3	Operation = Flow-through	Duration (min) = 8	Liquid Temperature (C) = 36	H_c @ 36 C Acetone	D_l @ 24 C 9.5×10^{-6}	D_g @ 24 C 0.11	39	37	0	0.036	5.3	0.54	6.0	249	42	99	
			Liquid Flowrate (L/min) = 9.1	Ethyl Acetate	0.0080	9.5×10^{-6}	0.092	24	21	0	0.059	11	1.2	4.9	205	42	102
			Gas Flowrate (L/min) = 359	Toluene	0.38	9.1×10^{-6}	0.085	6.7	4.1	0	0.037	38	4.5	4.8	198	42	94
			Shower Stall/Bathtub Volume (L) = 1745	Ethylbenzene	0.58	8.4×10^{-6}	0.077	5.9	3.6	0	0.022	39	4.5	4.7	196	42	87
			Person Present = No	Cyclohexane	10	9.0×10^{-6}	0.088	2.3	1.3	0	0.0074	38	5.1	5.1	211	42	82
4	Operation = Flow-through	Duration (min) = 8	Liquid Temperature (C) = 25	H_c @ 25 C Acetone	D_l @ 24 C 9.5×10^{-6}	D_g @ 24 C 0.11	40	40	0	0.017	1.7	0.18	2.4	159	66	102	
			Liquid Flowrate (L/min) = 6.1	Ethyl Acetate	0.0050	9.5×10^{-6}	0.092	25	24	0	0.029	4.5	0.32	1.3	86	66	103
			Gas Flowrate (L/min) = 350	Toluene	0.27	9.1×10^{-6}	0.085	5.2	4.0	0	0.013	22	1.6	1.7	110	66	95
			Shower Stall/Bathtub Volume (L) = 1745	Ethylbenzene	0.32	8.4×10^{-6}	0.077	4.0	3.1	0	0.0077	22	1.5	1.6	106	66	92
			Person Present = No	Cyclohexane	7.2	9.0×10^{-6}	0.088	1.1	0.81	0	0.0029	22	1.7	1.7	110	66	96

Operating Conditions		Chemical Properties			Chemical Concentrations			Mass Transfer Parameters								
		H _c @ 36 C Chemical	D _i @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _g A (L/min)	k _g /k _I	Mass Closure (%)		
5	Operation =	Flow-through														
	Duration (min) =	8														
	Liquid Temperature (C) =	36	Acetone	0.0024	1.1 x 10 ⁻⁵	0.11	48	46	0	0.034	4.3	0.43	2.4	227	96	101
	Liquid Flowrate (L/min) =	6.1	Ethyl Acetate	0.0080	9.5 x 10 ⁻⁶	0.092	25	22	0	0.043	14	1.1	2.4	234	96	101
	Gas Flowrate (L/min) =	361	Toluene	0.38	9.1 x 10 ⁻⁶	0.085	6.0	4.2	0	0.023	30	2.2	2.2	214	96	107
	Shower Stall/Bathtub Volume (L) =	1745	Ethylbenzene	0.58	8.4 x 10 ⁻⁶	0.077	4.0	3.1	0	0.017	29	2.1	2.2	207	96	100
	Person Present =	No	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	1.1	0.77	0	0.0038	27	1.9	1.9	182	96	103

Operating Conditions		Chemical Properties			Chemical Concentrations			Mass Transfer Parameters								
		H _c @ 37 C Chemical	D _i @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _g A (L/min)	k _g /k _I	Mass Closure (%)		
6	Operation =	Flow-through														
	Duration (min) =	8														
	Liquid Temperature (C) =	37	Acetone	0.0025	1.1 x 10 ⁻⁵	0.11	40	38	0	0.033	4.8	0.46	4.2	211	50	101
	Liquid Flowrate (L/min) =	6.1	Ethyl Acetate	0.0084	9.5 x 10 ⁻⁶	0.092	23	21	0	0.049	10	0.79	2.7	135	50	105
	Gas Flowrate (L/min) =	365	Toluene	0.39	9.1 x 10 ⁻⁶	0.085	6.0	3.7	0	0.023	38	2.9	3.1	152	50	92
	Shower Stall/Bathtub Volume (L) =	1745	Ethylbenzene	0.59	8.4 x 10 ⁻⁶	0.077	5.9	3.7	0	0.015	38	2.9	3.0	151	50	85
	Person Present =	No	Cyclohexane	11	9.0 x 10 ⁻⁶	0.088	2.0	1.2	0	0.0038	41	3.2	3.2	161	50	85

STUDY: Howard, C.L.

Study year: 1998

Reference: Volatilization Rates of Chemicals from Drinking Water to Indoor Air. Ph.D. Dissertation. University of Texas at Austin, May 1988

Solution Methods: Method 3

Assumptions: None

Comments:

* = Could not be determined with available data.

Operating Conditions		Chemical Properties			Chemical Concentrations			Mass Transfer Parameters								
		H _c @ 24 C Chemical	D _i @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _g A (L/min)	k _g /k _I	Mass Closure (%)		
7	Operation =	Fill														
	Duration (min) =	8														
	Liquid Temperature (C) =	24	Acetone	0.0012	1.1 x 10 ⁻⁵	0.11	41	39	0	0.018	4.9	0.45	7.1	395	56	97
	Liquid Flowrate (L/min) =	9.1	Ethyl Acetate	0.0013	9.5 x 10 ⁻⁶	0.092	25	24	0	0.030	3.0	1.0	4.9	274	56	103
	Final Liquid Volume (L) =	73	Toluene	0.27	9.1 x 10 ⁻⁶	0.085	8.0	5.6	0	0.029	31	4.1	4.4	244	56	89
	Gas Flowrate (L/min) =	373	Ethylbenzene	0.31	8.4 x 10 ⁻⁶	0.077	9.8	6.7	0	0.020	33	4.4	4.6	257	56	82
	Shower Stall/Bathtub Volume (L) =	1745	Cyclohexane	7.1	9.0 x 10 ⁻⁶	0.088	3.1	1.8	0	0.0063	46	7.1	7.1	396	56	73

Operating Conditions		Chemical Properties			Chemical Concentrations			Mass Transfer Parameters								
		H _c @ 35 C Chemical	D _i @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _g A (L/min)	k _g /k _I	Mass Closure (%)		
8	Operation =	Fill														
	Duration (min) =	8														
	Liquid Temperature (C) =	35	Acetone	0.0022	1.1 x 10 ⁻⁵	0.11	43	40	0	0.031	5.2	0.53	9.3	253	27	98
	Liquid Flowrate (L/min) =	9.1	Ethyl Acetate	0.0077	9.5 x 10 ⁻⁶	0.092	24	23	0	0.045	5.3	1.4	8.3	228	27	106
	Final Liquid Volume (L) =	73	Toluene	0.36	9.1 x 10 ⁻⁶	0.085	6.2	4.0	0	0.036	30	5.3	5.8	159	27	93
	Gas Flowrate (L/min) =	379	Ethylbenzene	0.54	8.4 x 10 ⁻⁶	0.077	6.3	3.9	0	0.024	32	5.9	6.3	172	27	81
	Shower Stall/Bathtub Volume (L) =	1745	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	2.0	0.85	0	0.0074	47	11	11	311	27	68

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
9		H _c @ 36 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _i A (L/min)	k _g A (L/min)	k _g /k _i	Mass Closure (%)	
Operation =	Fill	Chemical			40	39	0	0.032	2.0	0.64	5.9	303	51	101	
Duration (min) =	8				23	22	0	0.044	3.1	1.5	5.3	269	51	107	
Liquid Temperature (C) =	36	Acetone	0.0024	1.1 x 10 ⁻⁵	0.11										
Liquid Flowrate (L/min) =	9.1	Ethyl Acetate	0.0080	9.5 x 10 ⁻⁶	0.092										
Final Liquid Volume (L) =	73	Toluene	0.38	9.1 x 10 ⁻⁶	0.085	6.3	4.5	0	0.037	31	3.7	3.8	193	51	101
Gas Flowrate (L/min) =	373	Ethylbenzene	0.58	8.4 x 10 ⁻⁶	0.077	5.4	3.8	0	0.024	32	3.8	4.0	202	51	93
Shower Stall/Bathtub Volume (L) =	1745	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	1.2	0.66	0	0.0074	46	7.4	7.4	376	51	87

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
10		H _c @ 23 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _i A (L/min)	k _g A (L/min)	k _g /k _i	Mass Closure (%)	
Operation =	Fill	Chemical			41	39	0	0.019	5.8	0.39	4.7	365	77	96	
Duration (min) =	12				26	25	0	0.032	3.1	0.71	2.7	208	77	104	
Liquid Temperature (C) =	23	Acetone	0.0011	1.1 x 10 ⁻⁵	0.11										
Liquid Flowrate (L/min) =	6.1	Ethyl Acetate	0.0046	9.5 x 10 ⁻⁶	0.092										
Final Liquid Volume (L) =	73	Toluene	0.26	9.1 x 10 ⁻⁶	0.085	6.8	4.9	0	0.034	29	2.6	2.7	208	77	101
Gas Flowrate (L/min) =	370	Ethylbenzene	0.30	8.4 x 10 ⁻⁶	0.077	7.3	5.1	0	0.023	31	2.7	2.8	220	77	88
Shower Stall/Bathtub Volume (L) =	1745	Cyclohexane	6.9	9.0 x 10 ⁻⁶	0.088	3.0	1.8	0	0.0078	43	4.4	4.4	344	77	84

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
11		H _c @ 35 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _i A (L/min)	k _g A (L/min)	k _g /k _i	Mass Closure (%)	
Operation =	Fill	Chemical			40	37	0	0.032	7.7	0.39	4.2	191	46	98	
Duration (min) =	11.4				23	22	0	0.047	7.0	1.0	3.8	175	46	108	
Liquid Temperature (C) =	35	Acetone	0.0022	1.1 x 10 ⁻⁵	0.11										
Liquid Flowrate (L/min) =	6.1	Ethyl Acetate	0.0077	9.5 x 10 ⁻⁶	0.092										
Final Liquid Volume (L) =	69	Toluene	0.37	9.1 x 10 ⁻⁶	0.085	5.0	3.5	0	0.026	30	2.7	2.8	129	46	106
Gas Flowrate (L/min) =	377	Ethylbenzene	0.56	8.4 x 10 ⁻⁶	0.077	4.2	3.0	0	0.015	29	2.5	2.6	121	46	96
Shower Stall/Bathtub Volume (L) =	1745	Cyclohexane	10	9.0 x 10 ⁻⁶	0.088	1.2	0.63	0	0.0041	46	5.4	5.4	245	46	75

STUDY: Howard, C.L.

Study year: 1998

Reference: Volatilization Rates of Chemicals from Drinking Water to Indoor Air. Ph.D. Dissertation. University of Texas at Austin, May 1988

Solution Methods: Method 4 for toluene, ethylbenzene, and cyclohexane

Method 5 for acetone and ethyl acetate

Assumptions: None

Comments: Stripping efficiencies for entries 12 - 14 based on gas-phase data.

* = Could not be determined with available data.

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
12		H _c @ 23 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _i A (L/min)	k _g A (L/min)	k _g /k _i	Mass Closure (%)
Operation =	Bathing	Chemical			40	39	0.021	0.0030	0.6	*	*	*	*	99
Duration (min) =	20				25	25	0.035	0.0023	1.6	*	*	*	*	100
Liquid Temperature (C) =	23	Acetone	0.0011	1.1 x 10 ⁻⁵	0.11									
Liquid Volume (L) =	73	Ethyl Acetate	0.0046	9.5 x 10 ⁻⁶	0.092									
Gas Flowrate (L/min) =	370	Toluene	0.26	9.1 x 10 ⁻⁶	0.085	4.9	5.1	0.037	3.8 x 10 ⁻¹	7.9	*	*	*	96
Shower Stall/Bathtub Volume (L) =	1745	Ethylbenzene	0.3	8.4 x 10 ⁻⁶	0.077	5.1	5.3	0.025	4.2 x 10 ⁻¹	5.1	*	*	*	100
Person Present =	No	Cyclohexane	6.9	9.0 x 10 ⁻⁶	0.088	1.8	1.9	0.009	0	4.7	*	*	*	99

KITCHEN SINK DATABASE

STUDY: Howard and Corsi
Study year: 1996
Reference: *Journal of the Air and Waste Management Association*, Vol. 46, 1996, pp. 830-837.
Solution Method: Method 6
Assumptions: C_g assumed to be negligible
 $C_{g,in} = 0$

Comments: Mass transfer values based on recirculating flow.

* = Could not be determined with available data.

Entry #	Operating Conditions		Chemical Properties				Chemical Concentrations				Mass Transfer Parameters					
											η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)
1	Aerator Type = None	Liquid Temperature (C) = 23	H_c @ 23 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)	
	Liquid Flowrate (L/min) = 4.8	Hydraulic Residence Time (min) = 10	Acetone	0.0011	1.1×10^{-5}	0.11	93	45	0	0	4.9	0.24	1.3	136	104	*
	Dishes = None	Toluene	0.26	9.1×10^{-6}	0.085	11	0.44	0	0	21	1.0	1.0	108	104	*	
	Cyclohexane	6.9×10^{-6}	0.088	7.2	0.18	0	0	24	1.2	1.2	125	104	*			
2	Aerator Type = None	Liquid Temperature (C) = 23	H_c @ 23 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)	
	Liquid Flowrate (L/min) = 7.9	Hydraulic Residence Time (min) = 6.3	Acetone	0.0011	1.1×10^{-5}	0.11	56	41	0	0	2.2	0.17	1.7	88	51	*
	Dishes = None	Toluene	0.26	9.1×10^{-6}	0.085	14	1.2	0	0	17	1.3	1.4	72	51	*	
	Cyclohexane	6.9×10^{-6}	0.088	12	0.74	0	0	19	1.5	1.5	77	51	*			
3	Aerator Type = Screen	Liquid Temperature (C) = 23	H_c @ 23 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)	
	Liquid Flowrate (L/min) = 4.8	Hydraulic Residence Time (min) = 10	Acetone	0.0011	1.1×10^{-5}	0.11	70	53	0	0	1.7	0.080	1.0	41	43	*
	Dishes = None	Toluene	0.26	9.1×10^{-6}	0.085	9.4	0.84	0	0	13	0.65	0.7	30	43	*	
	Cyclohexane	6.9×10^{-6}	0.088	7.7	0.30	0	0	19	0.90	0.9	38	43	*			
4	Aerator Type = Screen	Liquid Temperature (C) = 23	H_c @ 23 C Chemical	D_l @ 24 C (m^3_{liq}/m^3_{gas})	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure (%)	
	Liquid Flowrate (L/min) = 7.9	Hydraulic Residence Time (min) = 6.3	Acetone	0.0011	1.1×10^{-5}	0.11	58	49	0	0	1.1	0.090	1.6	44	27	*
	Dishes = None	Toluene	0.26	9.1×10^{-6}	0.085	12	1.5	0	0	14	1.2	1.4	37	27	*	
	Cyclohexane	6.9×10^{-6}	0.088	8.4	0.64	0	0	18	1.4	1.4	38	27	*			

5	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
	Aerator Type =	Bubble Aerator		H_c @ 23 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l
Liquid Temperature (C) =	23	Chemical													
Liquid Flowrate (L/min) =	4.8	Acetone	0.0011	1.1×10^{-5}	0.11	54	42	0	0	1.4	0.065	1.8	31	18	*
Hydraulic Residence Time (min) =	10	Toluene	0.26	9.1×10^{-6}	0.085	6.5	0.11	0	0	23	1.1	1.3	24	18	*
Dishes =	None	Cyclohexane	6.9	9.0×10^{-6}	0.088	4.2	0.010	0	0	33	1.6	1.6	28	18	*

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters							
Aerator Type =	Bubble Aerator	Chemical (m ³ _{liq} /m ³ _{gas})	H _c @ 23 C	D _i @ 24 C	D _g @ 24 C	C _{i,in}	C _{i,out}	C _{g,in}	C _{g,end}	η	K _{L,A}	k _A	k _{g,A}	k _{g/k_i}	Mass Closure	
Liquid Temperature (C) =	23		(cm ² /sec)	(cm ² /sec)		(mg/L)	(mg/L)	(mg/L)	(mg/L)	(%)	(L/min)	(L/min)	(L/min)	(%)		
Liquid Flowrate (L/min) =	6.3		Acetone	0.0011	1.1 × 10 ⁻⁵	0.11	56	45	0	0	1.5	0.090	2.4	43	18	*
Hydraulic Residence Time (min) =	8.1		Toluene	0.26	9.1 × 10 ⁻⁶	0.085	7.0	0.2	0	0	22	1.4	1.7	31	18	*
Dishes =	None		Cyclohexane	6.9	9.0 × 10 ⁻⁶	0.088	4.3	0.013	0	0	35	2.2	2.2	41	18	*

Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
Aerator Type =	Bubble Aerator		H_c @ 23 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure
Liquid Temperature (C) =	23	Chemical													(%)
Liquid Flowrate (L/min) =	7.9	Acetone	0.0011	1.1×10^{-5}	0.11	58	54	0	0	1.6	0.13	3.6	63	18	*
Hydraulic Residence Time (min) =	6.3	Toluene	0.26	9.1×10^{-6}	0.085	9.8	2.8	0	0	23	1.9	2.3	41	18	*
Dishes =	None	Cyclohexane	6.9	9.0×10^{-6}	0.088	7.2	0.70	0	0	44	3.5	3.5	62	18	*

8	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Aerator Type =	Bubble Aerator		H_c @ 23 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$	$C_{l,out}$	$C_{g,in}$	$C_{g,end}$	η	$K_L A$	k_A	$k_g A$	k_g/k_l	Mass Closure
Liquid Temperature (C) =	23	Chemical					(mg/L)	(mg/L)	(mg/L)	(mg/L)	(%)	(L/min)	(L/min)	(L/min)	(%)	
Liquid Flowrate (L/min) =	4.8	Acetone	0.0011	1.1×10^{-5}	0.11	68	57	0	0	1.3	0.060	2.1	29	14	*	
Hydraulic Residence Time (min) =	10	Toluene	0.26	9.1×10^{-6}	0.085	5.0	2.8	0	0	24	1.2	1.5	21	14	*	
Dishes =	Yes	Cyclohexane	6.9	9.0×10^{-6}	0.088	3.8	0.015	0	0	40	1.9	1.9	26	14	*	

9	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Aerator Type =	Bubble Aerator		H_c @ 23 C (m^3_{liq}/m^3_{gas})	D_l @ 24 C (cm^2/sec)	D_g @ 24 C (cm^2/sec)	$C_{l,in}$ (mg/L)	$C_{l,out}$ (mg/L)	$C_{g,in}$ (mg/L)	$C_{g,end}$ (mg/L)	η (%)	$K_L A$ (L/min)	k_A (L/min)	$k_g A$ (L/min)	k_g/k_l	Mass Closure
Liquid Temperature (C) =	23	Chemical														
Liquid Flowrate (L/min) =	6.3	Acetone	0.0011	1.1×10^{-5}	0.11		81	59	0	0	3.4	0.21	2.8	106	38	*
Hydraulic Residence Time (min) =	8.1	Toluene	0.26	9.1×10^{-6}	0.085		8.1	0.44	0	0	26	1.6	1.8	68	38	*
Dishes =	Yes	Cyclohexane	6.9	9.0×10^{-6}	0.088		4.2	0.020	0	0	48	2.9	2.9	112	38	*

STUDY: Wooley, Nazaroff, and Hodgson
Study year: 1990
Reference: *Journal of the Air and Waste Management Association*, Vol. 40, 1990, pp.1114-1120
Solution Method: Method 8
Assumptions: Only significant mass transfer occurring due to wash solution with added ethanol.
Comments: There is not enough information given to consider additional emissions due to rinsing of dishes.
 Mass closure values based on numbers given in paper.

* = Could not be determined with available data.

		Operating Conditions			Chemical Properties				Chemical Concentrations				Mass Transfer Parameters					
10		Aerator Type =	unknown	H _c @ 23 C	D _l @ 24 C	D _g @ 24 C	C _{l,in}	C _{l,out}	C _{g,in}	C _{g,end}	η	K _L A	k _l A	k _g A	k _g /k _l	Mass Closure		
		Liquid Temperature (C) =	43	Chemical	(m ³ _{liquid} /m ³ _{gas})	(cm ² /sec)	(cm ² /sec)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(%)	(L/min)	(L/min)	(L/min)	(%)		
		Liquid Volume (L) =	7.6	Ethanol	0.0012	1.3 × 10 ⁻⁵	0.12	113	101	0	0	11	0.084	*	*	*	94	
		Duration (min) =	10	Ethanol	0.0012	1.3 × 10 ⁻⁵	0.12	113	105	0	0	7.1	0.055	*	*	*	96	
		Dishes =	Yes	Ethanol	0.0012	1.3 × 10 ⁻⁵	0.12	113	99	0	0	12	0.10	*	*	*	92	

		Operating Conditions			Chemical Properties				Chemical Concentrations				Mass Transfer Parameters					
11		Aerator Type =	unknown	H _c @ 23 C	D _l @ 24 C	D _g @ 24 C	C _{l,in}	C _{l,out}	C _{g,in}	C _{g,end}	η	K _L A	k _l A	k _g A	k _g /k _l	Mass Closure		
		Liquid Temperature (C) =	55	Chemical	(m ³ _{liquid} /m ³ _{gas})	(cm ² /sec)	(cm ² /sec)	(mg/L)	(mg/L)	(mg/L)	(mg/L)	(%)	(L/min)	(L/min)	(L/min)	(%)		
		Liquid Volume (L) =	7.6	Ethanol	*	1.3 × 10 ⁻⁵	0.12	278	279	0	0	-0.4	-5.1 × 10 ⁻⁴	*	*	*	106	
		Duration (min) =	70	Ethanol	*	1.3 × 10 ⁻⁵	0.12	278	283	0	0	-1.8	-0.0020	*	*	*	106	
		Dishes =	Yes	Ethanol	*	1.3 × 10 ⁻⁵	0.12	278	278	0	0	0	0	*	*	*	105	

WASHING MACHINE DATA BASE

STUDY: Howard, C.L.
Study year: 1998
Reference: *Journal of the Air and Waste Management Association*, Vol. 48, p. 907
Solution Method: Method 3
Assumptions: None
Comments: One gas sample collected for duration of experiment and one gas sample collected at end of experiment
Values of k_g/k_1 based solely on toluene, ethylbenzene, and cyclohexane data.

* = Could not be determined with available data.

STUDY: Howard, C.L.
Study year: 1998
Reference: *Volatilization Rates of Chemicals from Drinking Water to Indoor Air.* Ph.D. Dissertation. University of Texas at Austin, May 1988
Solution Method: Method 4 for toluene, ethylbenzene, and cyclohexane.
Method 5 for acetone and ethyl acetate.

Assumptions:

Comments:

* = Could not be determined with available data.

STUDY: Shepherd, Kemp, and Corsi

Study year: 1996

Reference: *Journal of the Air and Waste Management Association*, Vol. 46, No. 7, 1996, pp. 631-642.

Solution Method: Method 8. Stripping efficiencies based on predicted $C_{I,end}$ values using $K_L A$ values.

Assumptions: $C_{q,\text{in}} = C_q = 0$.

Comments: K_A values are equal to the total liquid volume multiplied by the K_a values reported in the paper, where a equals A/V.

* = Could not be determined with available data.

STUDY: Wooley, Nazaroff, and Hodgson

Study year: 1990

Reference: *Journal of the Air and Waste Management Association*, Vol. 40, 1990, pp. 1114-1120

Solution Method: Not enough information given to solve K_LA.

Stripping efficiency values based on mass of ethanol added to wash water and mass of ethanol remaining after operation.

Assumptions: $C_{g,in} = 0$.

Comments: Mass closure values from paper.

* = Could not be determined with available data.

DISHWASHER DATABASE

STUDY: Howard-Reed, C., Corsi, R., and Moya, J.
Study year: 1999
Reference: *Environmental Science and Technology*, Vol. 33, pp. 2266-2272.
Solution Method: Method 4
Assumptions: $C_{g,in} = 0$, unless otherwise given.
Comments: # = initial liquid-phase concentration based on average of duplicate samples with a relative difference greater than 20%, but no more than 36%. Mass closure is average over four time periods within experiment.

* = Could not be determined with available data.

Entry #	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
										η (%)	K _L A (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_I} (%)	Mass Closure	
1	Cycle Type =	Rinse	Chemical	H _c @ 43 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	50#	7.0	*	*	*	95
	Duration (min) =	10		0.0034	1.1 x 10 ⁻⁵	0.11						*	*	*	90	
	Liquid Temperature (C) =	43		Acetone	0.0034	1.1 x 10 ⁻⁵						97#	33	*	*	
	Liquid Volume (L) =	7.4		Toluene	0.46	9.1 x 10 ⁻⁶	0.085					97#	31	*	*	
	Headspace Volume (L) =	181		Ethylbenzene	0.80	8.4 x 10 ⁻⁶	0.077					100#	45	48	*	
	Ventilation Rate (L/min) =	5.7		Cyclohexane	13	9.0 x 10 ⁻⁶	0.088					100#	45	48	*	
2	Dishes Present =	No					100#					45	48	*	95	
	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Cycle Type =	Rinse	Chemical	H _c @ 42 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_I} (%)	Mass Closure
	Duration (min) =	10		0.0032	1.1 x 10 ⁻⁵	0.11						34	4.2	*	*	94
	Liquid Temperature (C) =	42		Acetone	0.0032	1.1 x 10 ⁻⁵	0.11					96	30	*	*	91
	Liquid Volume (L) =	7.4		Toluene	0.44	9.1 x 10 ⁻⁶	0.085					97	32	*	*	86
	Headspace Volume (L) =	181		Ethylbenzene	0.75	8.4 x 10 ⁻⁶	0.077					100	49	49	*	82
	Ventilation Rate (L/min) =	5.7		Cyclohexane	12	9.0 x 10 ⁻⁶	0.088					100	49	49	*	
3	Dishes Present =	Yes					100					49	49	*		
	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Cycle Type =	Rinse	Chemical	H _c @ 39 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_I} (%)	Mass Closure
	Duration (min) =	10		0.0028	1.1 x 10 ⁻⁵	0.11						43	5.8	*	*	93
	Liquid Temperature (C) =	39		Acetone	0.0028	1.1 x 10 ⁻⁵	0.11					97	32	*	*	91
	Liquid Volume (L) =	7.4		Toluene	0.42	9.1 x 10 ⁻⁶	0.085					98	35	*	*	87
	Headspace Volume (L) =	181		Ethylbenzene	0.68	8.4 x 10 ⁻⁶	0.077					100	58	58	*	83
	Ventilation Rate (L/min) =	5.7		Cyclohexane	12	9.0 x 10 ⁻⁶	0.088					100	58	58	*	
4	Dishes Present =	Yes					100					58	58	*		
	Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters						
	Cycle Type =	Wash	Chemical	H _c @ 43 C (m ³ _{liq} /m ³ _{gas})	D _i @ 24 C (cm ² /sec)	D _g @ 24 C (cm ² /sec)	C _{i,in} (mg/L)	C _{i,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _A (L/min)	k _{gA} (L/min)	k _{g/k_I} (%)	Mass Closure
	Duration (min) =	10		0.0034	1.1 x 10 ⁻⁵	0.11						37	5.1	*	*	92
	Liquid Temperature (C) =	43		Acetone	0.0034	1.1 x 10 ⁻⁵	0.11					96	30	*	*	99
	Liquid Volume (L) =	7.4		Toluene	0.46	9.1 x 10 ⁻⁶	0.085					97	33	*	*	93
	Headspace Volume (L) =	181		Ethylbenzene	0.81	8.4 x 10 ⁻⁶	0.077					100#	51	51	*	87
	Ventilation Rate (L/min) =	5.7		Cyclohexane	13	9.0 x 10 ⁻⁶	0.088					100#	51	51	*	
	Dishes Present =	No					100#					51	51	*		

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Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
Cycle Type =	Wash	H _c @ 55 C Chemical	D _l @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _l A (L/min)	k _g A (L/min)	k _g /k _l	Mass Closure (%)
Liquid Temperature (C) =	55	Acetone	0.0061	1.1 × 10 ⁻⁵	0.11	44	28	0.052	0.48	37	4.9	*	*	100
Liquid Volume (L) =	7.4	Toluene	0.62	9.1 × 10 ⁻⁶	0.085	9.9	0.34	0.010	0.29	97	31	*	*	98
Headspace Volume (L) =	181	Ethylbenzene	1.4	8.4 × 10 ⁻⁶	0.077	10	0.25	0.008	0.21	97	34	*	*	90
Ventilation Rate (L/min) =	5.7	Cyclohexane	18	9.0 × 10 ⁻⁶	0.088	5.1	0.014	0.004	0.080	100	47	46	*	85
Dishes Present =	Yes													

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Operating Conditions		Chemical Properties			Chemical Concentrations				Mass Transfer Parameters					
Cycle Type =	Wash	H _c @ 53 C Chemical	D _l @ 24 C (m ³ _{liq} /m ³ _{gas})	D _g @ 24 C (cm ² /sec)	C _{l,in} (mg/L)	C _{l,out} (mg/L)	C _{g,in} (mg/L)	C _{g,end} (mg/L)	η (%)	K _L A (L/min)	k _l A (L/min)	k _g A (L/min)	k _g /k _l	Mass Closure (%)
Liquid Temperature (C) =	53	Acetone	0.0056	1.1 × 10 ⁻⁵	0.11	60	36	0.008	0.48	40 [#]	5.2	*	*	97
Liquid Volume (L) =	7.4	Toluene	0.6	9.1 × 10 ⁻⁶	0.085	15	0.48	0.003	0.26	97 [#]	35	*	*	88
Headspace Volume (L) =	181	Ethylbenzene	1.3	8.4 × 10 ⁻⁶	0.077	17	0.41	0.0020	0.19	98 [#]	37	*	*	82
Ventilation Rate (L/min) =	5.7	Cyclohexane	17	9.0 × 10 ⁻⁶	0.088	8.5	0.026	0	0.092	100 [#]	55	54	*	84
Dishes Present =	Yes													